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Synthesis of mesityl oxide π-complexes with metals of chromium subgroup and with iron. Theoretical and experimental investigation of the ligand dissociation energy

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Abstract

At the use of photochemical and thermochemical activation new π-complexes of chromium, molybdenum, and tungsten were prepared containing in the coordination sphere η2- and η4-molecules of 4-methyl-3-penten-2-one. Nonempirical methods were applied to calculation of the energy parameters of the coordinated molecules, and the factors governing the η2- and η4-coordination of the oxodiene system were established. A thermochemical study was performed on the 4-methyl-3-penten-2-one η4-coordination product with carbonyl metal core. A scheme of the thermal decomposition was suggested for the iron (0) η 4-(4-methyl-3-pen-en-2-one)tricarbonyl.

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